

John K. Gibson

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Education

Ph.D. in Physical Chemistry (GPA = 3.99/4.00), University of California, Berkeley, 1983
Dissertation: “Thermochemistry of Acid-Base Stabilized Transition Metal Alloys by Carbide and Nitride Equilibria, and Knudsen Effusion Vapor Pressures.” Advisor: Leo Brewer

B.A. in Chemistry with a minor in Mathematics (GPA = 3.96/4.00), Boston University, 1979
Summa cum Laude with Distinction
Distinction Thesis: “Low-Temperature Thermal Effects in Li/ND₃ Systems.” Advisor: Lowell Coulter

Professional Experience

2007-Present: Senior Scientist, Lawrence Berkeley National Laboratory
2000-2007: Senior Research Staff, Oak Ridge National Laboratory
1986-2000: Research Staff, Oak Ridge National Laboratory
1983-1986: Research Associate, Oak Ridge National Laboratory
1983: Postdoctoral Research Associate, Lawrence Berkeley National Laboratory
1981-1983: Graduate Student Research Associate, Lawrence Berkeley National Laboratory
1979-1981: Graduate Student Teaching Assistant, UC Berkeley

Research

The primary research focus is on utilizing gas-phase ion chemistry and spectroscopy to elucidate the chemistry of the members of the first half of the actinide series, Th, Pa, U, Np, Pu, Am and Cm. Among the aspects of the chemistry of these elements that are of particular interest and importance are the participation of the quasi-valence 5f electrons in chemical bonding, and the variety of readily accessible oxidation states, e.g., Pu(III/IV/V/VI). Gas-phase chemistry provides fundamental insights for simple systems unperturbed by interactions with solvent or other neighboring atoms and molecules. This simplicity renders the studied species particularly amenable to theoretical computations, which serve to both elucidate the experimental observations and provide a basis to validate and reliably extend theoretical methodologies. Many of the studied gas-phase complexes provide a link between condensed phase and gas phase, where species can be probed in greater detail and provide insights into condensed phase behavior. Most of the experimental approaches employ mass spectrometry, particularly ion trap mass spectrometry in which trapped ions can be systematically manipulated and examined. Some properties being explored and methodologies being employed are given below.

- Gas-phase ion-molecule reactions
- Role of 5f electrons in molecular actinide chemistry
- Actinide molecular bond energies and ionization energies
- Synthesis of novel complexes by collision induced dissociation of clusters
- Catalytic processes mediated by bare and ligated actinide ions
- Interplay between theoretical and experimental thermodynamics and mechanisms
- Electrospray ionization of actinide complexes
- Actinide bio-inorganic chemistry from the bottom up
- Elucidating solution chemistry: hydration, solvation, hydrolysis and complexation

- Gas-phase cluster synthesis by laser ablation of solids
- Infrared spectroscopy of gas-phase metal ion complexes
- Highly charged metal ions from solution to gas
- Electron transfer dissociation of multiply charged metal cation complexes

Selected Recent Publications (128 total)

“Experimental and Theoretical Studies on the Fragmentation of Gas-Phase Uranyl-, Neptunyl- and Plutonyl-Diglycolamide Complexes,” Y. Gong, H.-S. Hu, L. Rao, J. Li, J. K. Gibson, *J. Phys. Chem. A*, Web-published on Sept. 9, 2013 (DOI: 10.1021/jp4076977)

“A Tetrapositive Metal Ion in the Gas Phase: Th⁴⁺ Coordinated by Neutral Tridentate Ligands,” Y. Gong, H. S. Hu, G. Tian, L. Rao, J. Li, J. K. Gibson, *Angew. Chem. Int. Ed.* 52 (2013) 6885-6888.

“Formation and Characterization of the Uranyl-SO₂ Complex, UO₂(CH₃SO₂)(SO₂)⁻,” Y. Gong, J. K. Gibson, *J. Phys. Chem. A* 117 (2013) 783-787.

“Proton Transfer in Th(IV) Hydrate Clusters: A Link to Hydrolysis of Th(OH)₂²⁺ to Th(OH)₃⁺ in Aqueous Solution,” P. X. Rutkowski, M. C. Michelini, J. K. Gibson, *J. Phys. Chem A* 117 (2013) 451-459.

“The Origins of Faster Oxo-Exchange for Uranyl(V) versus Plutonyl(V),” D. Rios, M. C. Michelini, A. F. Lucena, J. Marçalo, J. K. Gibson, *J. Am. Chem. Soc.*, 134 (2012) 15488-15496.

“Gas-Phase Uranyl, Neptunyl and Plutonyl: Hydration and Oxidation Studied by Experiment and Theory,” D. Rios, M. C. Michelini, A. F. Lucena, J. Marçalo, T. H. Bray, J. K. Gibson, *Inorg. Chem.*, 51 (2012) 6603-6614.

“Activation of Gas-Phase Uranyl Diacetone Alcohol Coordination Complexes by Spectator Ligand Addition,” D. Rios, J. K. Gibson, *Eur. J. Inorg. Chem.* (2012) 1054-1060.

“Lanthanide Gas-Phase Lanthanide Chloride Clusters: Relationships among ESI Abundances and DFT Structures and Energetics,” P. X. Rutkowski, M. C. Michelini, J. K. Gibson, *Phys. Chem. Chem. Phys.* 13 (2012) 1065-1977.

“Electron Transfer Dissociation of Dipositive Uranyl and Plutonyl Coordination Complexes,” D. Rios, P. X. Rutkowski, J. K. Gibson, M. J. Van Stipdonk, *J. Mass Spectrom.* 46 (2011) 1247-1254.

“Gas-Phase Coordination Complexes of U^{VI}O₂²⁺, Np^{VI}O₂²⁺, and Pu^{VI}O₂²⁺ with Dimethylformamide,” P. X. Rutkowski, D. Rios, D. K. Shuh, T. H. Bray, J. K. Gibson, M. J. Van Stipdonk, *J. Am. Soc. Mass Spectrom.* 22 (2011) 2042-2048.

“Gas-Phase Reactions of Doubly Charged Actinide Cations with Alkanes and Alkenes - Probing the Chemical Activity of 5f Electrons From Th to Cm,” J. Marçalo, M. Santos, J.K. Gibson, *Phys. Chem. Chem. Phys.* 13 (2011) 19322-18329.

“Actinide sulfides in the gas phase: experimental and theoretical studies of the thermochemistry of AnS (An = Ac, Th, Pa, U, Np, Pu, Am and Cm),” C. C. L. Pereira, C. J Marsden, J. Marçalo, J. K. Gibson, *Phys. Chem. Chem. Phys.* 13 (2011) 12940-12958.

“Gas-Phase Coordination Complexes of Dipositive Plutonyl and Uranyl Ions,” D. Rios, P. X. Rutkowski, M. J. Van Stipdonk, J. K. Gibson, *Inorg. Chem.* 50 (2011) 4781-4790.

“Gas-phase reactions of the bare Th²⁺ and U²⁺ ions with small alkanes, CH₄, C₂H₆ and C₃H₈: An experimental and theoretical study of elementary organoactinide chemistry,” E. Di Santo, M. Santos, M. C. Michelini, J. Marçalo, N. Russo, J. K. Gibson, *J. Am. Chem. Soc.* 211 (2011) 1955-1970.

“Gas-phase reactions of uranate ions, UO₂⁻, UO₃⁻, UO₄⁻ and UO₄H, with methanol: A convergence of experiment and theory,” M. C. Michelini, J. Marçalo, N. Russo, J. K. Gibson, *Inorg. Chem.* 49 (2010) 3836-3850.

Professional Recognition, Honors, and Service

2013: Organizer for ACS Seaborg Award Symposium in Honor of Richard G. Haire
1983 – Present: Principal Investigator, DOE/BES Heavy Element Chemistry Program
2001 – Present: Guest Scientist, Instituto Tecnológico e Nuclear, Portugal
2010: Symposium Organizer and Proceedings Lead Editor, MRS National Meeting
2003: Chair, East Tennessee Section, American Chemical Society
2002: Consultant, International Atomic Energy Agency, Vienna
2001: On-site reviewer, DOE/BES Chemical Sciences Research Programs at LBNL
1999: ORNL “Author of the Year”
1999: ORNL Technical Achievement Award for gas-phase actinide ion chemistry
1998: ORNL Chemical and Analytical Sciences Division Research Accomplishment Award for gas-phase organoactinide chemistry
1997: ORNL Chemical and Analytical Sciences Division R&D Accomplishment Award for development of actinide laser ablation mass spectrometer
1988: ORNL Technical Achievement Award for determination of the sublimation enthalpy of Fm
1979: Boston University Chemistry Department Outstanding Senior Undergraduate Award
1978: Phi Beta Kappa

Reviewer for: *J. Am. Chem. Soc.*, *J. Phys. Chem.*, *Inorg. Chem.*, *Angew. Chem.*,
Organometallics, *Chem. Materials*, *Chem. Eur. J.*, *Int. J. Mass Spectrometry*,
J. Am. Soc. Mass Spectrometry, *J. Mass Spectrometry*, *Radiochimica Acta*,
J. Nuclear Materials, *Chem. Phys. Lett.*, *Int. J. Chem. Kinetics*; *Spectrochim. Acta*,
Applied Spectroscopy; *Dalton Trans.*; *J. Chem. Phys.*; *Phys. Chem. Chem. Phys.*

Member: American Chemical Society; American Association of Arts and Sciences; Materials Research Society; American Society for Mass Spectrometry

Research Supervision:

Yu Gong, Postdoctoral Fellow, LBNL, 2012-present
Daniel Rios, Postdoctoral Fellow, LBNL, 2010-2012
Philip Rutkowski, Postdoctoral Fellow, LBNL, 2009-2011
Travis Bray, Postdoctoral Fellow, LBNL, 2008-2010
Paul Momoh, Postdoctoral Fellow, LBNL, 2008-2009

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